Revealing the Molecular Packing in Small Organic Semiconductor Films with Synchrotron X-ray Scattering

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It is a well-known fact that the exact arrangement of small organic semiconductor molecules in polycrystalline thin films determines the film's intrinsic charge transport properties and consequently the electrical performance in thin-film devices such as organic thin film transistors (OTFTs). Grazing incidence X-ray scattering (GIXS) using a synchrotron light source can provide rich information about the molecular packing in polycrystalline films of small organic semiconductor molecules as thin as a fraction of a single monolayer. The combination of GIXS and advanced crystallographic refinement calculations allows us to obtain a detailed picture of the molecular packing at the entire semiconductor/dielectric interface, including self-assembled monolayer (SAM) dielectric surface modifications.

The utility of this approach is highlighted with several examples, including very high-performance printed thin films of 6,13-bis(triisopropylsilylethynyl) pentacene (TIPS-pentacene). By careful control of the printing condition, the π - π stacking distance between the TIPS-pentacene molecules in printed thin films can be significantly reduced from the bulk value of 3.3Å to 3.1Å, with the charge carrier mobility simultaneously increasing from 0.4 cm^2/Vs to a record high mobility of 4.6 cm^2/Vs.